# What is the skill of ocean tracers in reducing uncertainties about ocean diapycnal mixing and projections of the Atlantic Meridional Overturning Circulation?

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### Abstract

Current projections of the oceanic response to anthropogenic climate forcings are uncertain. Two key sources of these uncertainties are (i) structural errors in current Earth system models and (ii) imperfect knowledge of model parameters. Ocean tracers observations have the potential to reduce these uncertainties. Previous studies typically consider each tracer separately, neglect potentially important statistical properties of the system, or use methods that impose rather daunting computational demands. Here we extend and improve upon a recently developed approach using horizontally averaged vertical profiles of chlorofluorocarbon (CFC-11), radiocarbon ( $\Delta^{14}$ C), and temperature (T) observations to reduce model parametric and structural uncertainties. Our method estimates a joint probability density function, which considers cross-tracer correlations and spatial 11 autocorrelations of the errors. We illustrate this method by estimating two model param-12 eters related to the vertical diffusivity, the background vertical diffusivity and the upper 13 Southern Ocean mixing. We show that enhancing the upper Southern Ocean mixing in 14 the model improves the representations of ocean tracers, as well as improves hindcasts of 15 the Atlantic Meridional Overturning Circulation (AMOC). The most probable value of the background vertical diffusivity in the pelagic pycnocline is between 0.1-0.2 cm<sup>2</sup>s<sup>-1</sup>.

- According to the statistical method, observations of  $\Delta^{14}$ C reduce the uncertainty about
- 19 the background vertical diffusivity the most followed by CFC-11 and T. Using all three
- tracers jointly reduces the model uncertainty by 40%, more than each tracer individu-
- 21 ally. Given several important caveats, we illustrate how the reduced model parametric
- <sup>22</sup> uncertainty improves probabilistic projections of the AMOC.

### 1. Introduction

The North Atlantic Overturning Circulation (AMOC) is a key component of the climate system [Munk & Wunsch, 1998]. Past changes in the AMOC intensity are associated with considerable changes in global scale temperature and precipitation patterns [McManus et al., 2004]. Anthropogenic climate forcings may trigger an AMOC threshold response, with potentially serious impacts on natural systems and human welfare [Patwardhan, 2007; Keller et al., 2000]. Current AMOC model predictions are deeply uncertain [Zickfeld et al., 2007; Meehl et al., 2007].

Tracer observations such as chlorofluorocarbon-11 (CFC-11) and radiocarbon ( $\Delta^{14}C$ )
provide information on the ventilation rate and advective properties in the ocean on timescales ranging from decadal to centennial that can be used for evaluating the skill of climate
models in simulating the ocean circulation [Doney et al., 2004]. A better representation
of these processes in models can possibly improve AMOC projections.

A key variable for determining ocean circulation properties in models is the vertical ocean diffusivity  $(K_v)$ . Changing this value in model simulations has a large impact on oceanic heat storage and transport, uptake of ocean tracers such as  $CO_2$  [Sokolov et al., 1998], and on the work necessary to lift the abyssal waters through stratification (that closes the MOC circulation) [Wunsch & Ferrari, 2004]. This variable is highly uncertain [Munk & Wunsch, 1998], and it is sometimes tuned in models to generate a realistic AMOC strength [Gao et al., 2003]. In addition, this parameter value affects the existence of multiple states of the MOC in model simulations [Schmittner & Weaver, 2001].

Various processes lead to mixing in the ocean such as shear or buoyancy forced turbulence, interactions of flow with topography, and double diffusion (differential molecular
diffusion of heat and salt). See  $Smyth \, \mathcal{E} \, Moum \, [2001]$  and  $Moum \, \mathcal{E} \, Smyth \, [2001]$  for reviews. Although General Circulation Models have been increasing their ability of parameterizing subgrid scale turbulent processes in the ocean ( $Bryan \, \mathcal{E} \, Lewis \, [1979]$ ;  $Pacanowski \, \mathcal{E} \, Philander \, [1981]$ ;  $Large \, et \, al. \, [1994]$ ;  $Ferrari \, et \, al. \, [2008]$ ), due to the complexity of
the problem and processes involved, most schemes are still highly simplified and parameterized. In Earth System Models of Intermediate Complexity (EMICs), the absence of
more complex parameterizations elevates the importance of the parameters related to  $K_v$ in order to fulfill the model necessity of turbulent mixing in simulating a realistic AMOC
strength.

Several studies [e.g. England, 1993; Gao et al., 2003] analyze the importance of the magnitude of the diffusivity strength and parameterization on the MOC structure and representations of tracers in ocean models. These studies are typically silent on the question of how much information is contained in the different types of observations. This is an important question, for example, to inform the design of AMOC observation and prediction systems [cf. Baehr et al., 2008; Keller et al., 2007].

Schmittner et al. [2009] discusses a relatively simple but computationally efficient method to estimate the background ocean diffusivity  $K_{bg}$  from the combination of spatially resolved ocean tracer observations considering both, observational and model errors. However, Schmittner et al. [2009] neglects the effects of cross-correlation between different tracers, which limits the number of tracers that can be combined in a joined probability density function. In another recent study, Bhat et al. [2009] estimates the posterior prob-

- ability distribution for  $K_{bg}$  using  $\Delta^{14}\mathrm{C}$  and CFC-11 observations. Their approach uses a
- Gaussian process emulator for the climate model and estimates the distribution of  $K_{bq}$
- via a Bayesian approach. While their kernel mixing based approach to constructing the
- emulator is flexible and efficient, it is conceptually complex and computationally highly
- demanding for routine use with more than two ocean tracers.
- Here we estimate the probability density function (pdf) of  $K_{bg}$  using three tracers si-
- multaneously. Our approach provides a fast and easy way to implement the methodology,
- enabling the routine use of information from several ocean tracers jointly, while still con-
- <sup>74</sup> sidering spatial autocorrelation as well as cross-correlation between residuals of different
- tracers. We demonstrate how neglecting cross-correlation and/or simplifying the mean
- function can compromise the accuracy of the estimation. We improve the treatment of
- uncertainties surrounding  $K_v$  in the model by considering the structural uncertainty about
- the upper Southern Ocean mixing  $(u_{-}K_{SO})$ . We show that an ensemble with enhanced
- Southern Ocean mixing is more consistent with the observations.
- Furthermore, we advance on previous work by quantifying and ranking the skill of the
- tracers CFC-11,  $\Delta^{14}$ C and temperature (T) to constrain the uncertainties in the model
- parameter  $K_{bq}$ . We demonstrate the potential utility of the considered observations to
- improve model predictions of the AMOC.

### 2. Methods

## 2.1. Earth System Model of Intermediate Complexity

- We use the University of Victoria Earth System Model of Intermediate Complexity
- (UVic 2.8; Weaver et al. [2001]). This model has been widely used in climate simulations
- 86 and models comparisons studies. In the UVic model, we parameterize the diapycnal

diffusivity as  $K_v = K_{tidal} + K_{SO} + K_{bg}$ , which consists of the diffusivity due to local dissipation of tidal energy and its resulting generation of turbulence and mixing  $(K_{tidal}, Simmons\ et\ al.\ [2004])$ , a parametrization for the vigorous mixing  $(K_{SO})$  observed in the Southern Ocean [e.g. Naveira Garabato et al., 2004], plus a background diffusivity  $K_{bg}$  that represents all other processes that lead to mixing, such as non-local dissipation of tidal energy, mesoscale eddy activity, double diffusion, hurricanes, interaction of flow with topography, and others.

The model accounts for increased mixing over rough topography based on the tidal mixing scheme of St. Laurent et al. [2002], and uses the Gent & McWilliams [1990] 95 eddy mixing parameterization. It is likely that  $K_{bg}$  is spatially and temporally variable in nature [Sriver et al., 2010], but due to a lack of a more explicit representation of the 97 processes and for simplicity we assume a constant value of  $K_{bg}$  everywhere. Note that  $K_{tidal}$  decays exponentially (with an e-folding depth of 500 m above the sea floor) such that it is unimportant in the pelagic pycnocline (i.e., away from the boundaries). However, 100 it is the value of  $K_{bg}$  in the pelagic pycnocline that is most important in determining 101 the large scale ocean circulation in models [c.f., Marotzke, 1997; Munk & Wunsch, 1998]. 102 For the Southern Ocean (south of 40S) parametrization, the vertical mixing is truncated at  $1 \text{ cm}^2/\text{s}$  as a lower bound  $(K_v > 1 \text{ cm}^2/\text{s})$ . The Southern Ocean is one of the most tempestuous oceans on earth, and these transient effects may produce strong turbulent mixing, specially in the upper Southern Ocean. In order to include uncertainties about the upper Southern Ocean mixing, we further divide the Southern Ocean mixing into upper 10  $(u_{-}K_{SO})$  and lower  $(l_{-}K_{SO})$  parts. Therefore,  $K_{SO} = u_{-}K_{SO} + l_{-}K_{SO}$ , where  $u_{-}K_{SO}$  is the Southern Ocean mixing in the upper 500 m, and  $l_{-}K_{SO}$  is the Southern Ocean mixing from 500m to the bottom of the water column.

We create two ensembles to analyze the uncertainty in two model parameters, the 11: background ocean diffusivity  $(K_{bg})$  and the upper Southern Ocean diffusivity  $(u_{-}K_{SO})$ . Each ensemble contains seven members, corresponding to a grid of the parameter  $K_{bg}$ 113 values of  $(0.05, 0.1, 0.15, 0.2, 0.3, 0.4, \text{ and } 0.5) \text{ cm}^2\text{s}^{-1}$ . The difference between the two 114 ensembles is that in the first one (ENSEMBLE 1), the enhanced SO mixing is only applied 115 in the lower part of the Southern Ocean, so in the upper SO the mixing is equal to the 116 rest of the pelagic areas of the upper ocean (with indices  $u_{-}K_{SO}=0$ ,  $l_{-}K_{SO}=1$ ), whereas 117 the second one (ENSEMBLE 2) uses an enhanced mixing in the entire column of the 118 Southern Ocean (with indices  $u_{-}K_{SO}=1$ ,  $l_{-}K_{SO}=1$ ). As we are not varying the parameter 119  $l_{-}K_{SO}$ , it is suppressed in the rest of the manuscript. 120

The ocean component in UVic is MOM2 [Pacanowski, 1995] with a  $1.8^{\circ} \times 3.6^{\circ}$  resolution in the horizontal and 19 depth levels. The atmospheric component is a one-layer atmospheric energy-moisture balance model, which does not apply flux correction and is forced by prescribed winds from the NCAR/NCEP climatology. Also included in the model are a thermodynamic sea-ice component, a terrestrial vegetation (TRIFFID), and an oceanic biogeochemistry based on the ecosystem model of  $Schmittner\ et\ al.\ [2005]$ .

A total of 47,600 model years was preformed, what makes UVic suitable for this kind of study. At first, the model is spun up from observed data fields as initial conditions for 3000 years (with a coupled carbon cycle for the last 1000 years) for each parameter value. It is then integrated from years 1800-2100 using historical and projected climate forcings (SRES-A1FI scenario), extended to the year 2200 following *Zickfeld et al.* [2008].

We modify the model to include non-CO<sub>2</sub> greenhouse gases, volcanic and sulfate forcings from *Sato et al.* [1993] and *Hansen & Sato* [2004]. Atmospheric sulfates data enter the model as gridded optical depth [*Koch et al.*, 1999], and follow the same rate of decrease as the CO<sub>2</sub> concentration after 2100.

### 2.2. Data

We focus on a subset of observations that have previously been shown to provide con-136 straints on the parameterization of  $K_v$  in ocean models: (i) temperature (T), (ii) chlo-137 rofluorocarbon 11 (CFC-11), and (iii) radiocarbon ( $\Delta^{14}$ C) observations [cf. Schmittner et al., 2009; Bhat et al., 2009; Toggweiler et al., 1989].  $\Delta^{14}$ C is defined as the  $^{14}$ C/ $^{12}$ C 139 ratio of air-sea fractionation-corrected data [Stuiver & Polach, 1977]. Each of the tracers in this subset has a different behavior, and can constrain  $K_v$  in different ways. The temperature observations constrain  $K_v$ , because  $K_v$  affects, for example, the shape of the thermocline as well as the penetration of the anthropogenic heat anomalies [Gnanade-143 sikan, 1999]. The  $\Delta^{14}$ C observations can constrain  $K_v$  in two main ways, because it has a natural and an anthropogenic component. The natural component can provide infor-145 mation of mixing rates (that are, in turn, a function of  $K_v$ ) in the order of centuries or 146 millennia. The anthropogenic component, which greatly increased during the 1950s and 147 1960s due to thermonuclear explosions, provides information on decadal time-scale. Here 148 we do not make distinction between natural and bomb 14C, thus we use its total con-149 centration. The anthropogenic tracer CFC-11 also constrains  $K_v$  on decadal time-scale, 150 because atmospheric emissions started in the 1930s. The solubility of CFCs in water is 151 dependent on the temperature. Considering CFC-11 and  $\Delta^{14}$ C jointly can provide new 152 insights into vertical oceanic mixing because they have very different forcing histories,

air-sea equilibration timescales and water solubility [Broecker & Peng, 1974; Ito et al., 2004, and the observation errors and signal-to-noise ratios of the two tracers are different. We analyze published data products for these three tracers [Locarnini et al., 2006; Key et al., 2004 and average the model hindcasts over the time the observations have been col-157 lected, i.e., 1990's for CFC-11 and  $\Delta^{14}$ C, and 1950-2000 for temperature. We interpolate 158 the observations to the model grid and the model output is restricted to the regions where 159 the data products are available. All considered ocean tracer observations are horizontally 160 averaged into global mean vertical profiles. Further, the probability distributions of the 161 model parameters, inferred from the information of ocean tracers profiles, are compared 162 with the distribution inferred from the climatological observations of the AMOC strength 163 at 24°N. For this purpose, we use the information of the AMOC strength calculated with 164 the inverse model of Lumpkin & Speer [2003], which is estimated as  $(17.6\pm2.7 \text{ Sy})$ . The 165 model ensembles are calibrated against observations using a Bayesian inference method. 166 We assume a Gaussian likelihood function and estimate the posterior probability of  $K_{bq}$ 167 and  $u_{-}K_{SO}$  given the observations through a Markov Chain Monte Carlo (MCMC) method [Metropolis et al., 1953]. Our method accounts for auto-correlations of the residuals, as 169 well as cross-correlation between residuals of different tracers. For this, a separable covariance matrix  $\Sigma$  is estimated. The inversion and the numerical implementation of the calibration procedure are detailed in the next subsection. Readers not interested in the 172 details of the statistical inversion technique can skip the next subsection without loss of 173 understanding. 174

### 2.3. Bayesian model inversion

The goal of Bayesian parameter estimation is to infer a probability distribution(s)  $p(\theta|O)$  representing the uncertainty in one (or more) climate model parameter  $\theta$ , conditional on a vector of observed data O. Here  $\theta$  are parameters  $K_{bg}$  and  $u_-K_{SO}$ , which are related to the vertical ocean diffusivity in UVic. The inferential procedure is based on a statistical model that relates the model parameters  $(\theta)$  to the observations (O) by way of the ensemble of model output  $M(\theta)$ . The statistical model used here assumes that the observations are randomly distributed around the model prediction, according to

$$O = M(\theta) + \epsilon \,, \tag{1}$$

where the error is a random variable drawn from a multivariate normal distribution

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$$\epsilon \sim N(\mu, \Sigma)$$
, (2)

with an unknown mean or bias term  $\mu$  and covariance matrix  $\Sigma$ . These distributional 183 parameters are estimated along with the model parameter  $\theta$ . The error term encompasses 184 all processes which may cause the observations to deviate from the model predictions, 185 including model structural error, unresolved variability in the climate system, and mea-186 surement error. We model these errors as random processes, approximated here by a 187 potentially correlated Gaussian probability function. 188 The error mean term  $\mu$  represents model bias, which is common for each observed 189 variable across ensemble members. Schmittner et al. [2009] assumed a bias which is constant with depth. Here we expand upon this form by using a general linear form that 19 varies with depth (z),  $\mu = az + b$ . This form improves the model fit as indicated by a exploratory data analysis in the next section. The covariance matrix, described later, captures the residual variability that is unaccounted by the linear bias term.

The above probability model describing the spread of observations about the model output defines a likelihood function  $L(O|\theta,\mu,\Sigma)$  for the data conditional on the model and covariance parameters:

$$L(O|\theta, \mu, \Sigma) = (2\pi)^{-N/2} |\Sigma|^{-1/2} \exp\left(-\frac{1}{2}\tilde{r}^T \Sigma^{-1}\tilde{r}\right),$$
 (3)

where  $\Sigma$  is a covariance matrix and  $\tilde{r} = O - M(\theta) - \mu$  are the bias-corrected data-model residuals.

Consider an ensemble M containing p runs of a climate model, where each run corresponds to a different value of a climate model parameter,  $\theta_k$ , k = 1, ..., p. For each ensemble member we analyze n ocean tracer profiles defined at d spatial locations (depths). The matrix  $\Sigma$  is  $nd \times nd$  specifying the covariance between n tracers at d locations (depths). Assuming separability,  $\Sigma$  can be approximated by a Kronecker product of two matrices:

$$\Sigma = \Sigma_T \otimes C_S + \Sigma_M \,, \tag{4}$$

where  $\Sigma_T$  corresponds to the  $n \times n$  cross-covariance matrix of the tracers, and  $C_S$  is
the  $d \times d$  spatial correlation matrix (in depth) respectively.  $\Sigma_M$  is the data measurement
error which we assume to be negligible compared to the other errors because of the spatial
aggregation of the data.

The cross-covariance matrix  $\Sigma_T$  depends on n(n-1)/2 cross-tracer correlation coefficients  $\rho_{ij}$  (since  $\rho_{ij} = \rho_{ji}$ ), and on residual standard deviations  $\sigma_i$  of the n individual tracers:

$$\Sigma_T = \begin{bmatrix} \sigma_1^2 & \sigma_1 \sigma_2 \rho_{12} & \dots & \sigma_1 \sigma_n \rho_{1n} \\ \sigma_2 \sigma_1 \rho_{21} & \sigma_2^2 & \dots & \sigma_2 \sigma_n \rho_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_n \sigma_1 \rho_{n1} & \dots & \dots & \sigma_n^2 \end{bmatrix} . \tag{5}$$

We model the spatial correlation  $C_S$  using a Gaussian correlation function, a special case of the Matérn class of covariance functions (see, for e.g., Stein [1999]). This function decays with distance between locations  $d_i$  and  $d_j$  with a correlation length scale  $\lambda$ , assumed to be the same for all tracers:

$$(C_S)_{ij} = \exp\left(-\frac{|d_i - d_j|^2}{\lambda^2}\right). \tag{6}$$

Given the property of the Kronecker product (see, for example,  $Lu \, \& \, Zimmerman$  [2005]), the multivariate normal likelihood function  $L(y, \theta)$  becomes:

$$L(O|\theta, \mu, \Sigma_T, C_S) = (2\pi)^{-N/2} (|\Sigma_T|^d |C_S|^n)^{-1/2} \exp\left[-\frac{1}{2}\tilde{r}^T (\Sigma_T^{-1} \otimes C_S^{-1})\tilde{r}\right],$$
 (7)

where N=nd is the total number of data points, and  $\tilde{r}_{=}[O_{1}-M_{1}-\mu_{1},\ldots,O_{n}-M_{n}-\mu_{n}]^{T}$  is the concatenated vector containing the misfit between the unbiased model predictions and the corresponding observations for the considered tracers. The Kronecker structure of Equation 4 allows the  $nd \times nd$  matrix  $\Sigma$  to be efficiently inverted by inverting the two smaller matrices  $\Sigma_{T}$   $(n \times n)$  and  $C_{S}$   $(d \times d)$ .

Once the probability model has been specified in the form of a likelihood function, the Bayes' theorem allows inference about the posterior distribution of  $\theta$ . The theorem states that the posterior probability of the unknown parameters is proportional to their prior

probability distribution, multiplied by the likelihood of the data, according to:

We draw 20,000 samples from the above posterior distribution by a Markov chain Monte

$$p(\theta, a, b, \sigma, \rho, \lambda | O) \propto L(O|\theta, a, b, \sigma, \rho, \lambda) p(\theta) p(a) p(b) p(\sigma) p(\rho) p(\lambda)$$
. (8)

Carlo (MCMC) algorithm. The MCMC algorithm jointly estimates the model parameters  $(\theta = K_{bg}, u_{-}K_{SO}), 2n$  bias coefficients  $(a_i \text{ and } b_i), n \text{ standard deviations } (\sigma_i), n(n-1)/2$ cross-tracer correlations  $(\rho_{ij})$ , and one correlation length  $(\lambda)$ . This is an improvement upon the methodology of Schmittner et al. [2009] which held all parameters but  $\theta$  fixed at 23 optimized values, and did not consider the uncertainty in the other parameters. Because 232 the model output is only defined on a discrete grid of values, the MCMC algorithm 233 proposes discrete jumps for the parameters  $\theta$  during its random walk through parameter 234 space, and continuous moves for all other parameters. 235 We choose a uniform prior  $p(\theta)$  for the model parameters  $K_{bg}$  and  $u_{-}K_{SO}$ . For the 236 correlation length we apply the lognormal prior  $\ln \lambda \sim N(5.5, 0.5^2)$ , such that the loga-237 rithm of  $\lambda$  is normally distributed with mean 5.5 and standard deviation 0.5. This prior 238 locates most of the probability mass of the distribution between 0 and 600 meters. We use 239 normal priors for the bias parameters  $a_i$  and  $b_i$ ,  $p(a_i)=N(0,(\sigma_i/\lambda)^2)$  and  $p(b_i)=N(0,\sigma_i^2)$ . For the estimate of individual tracers distributions, where the cross-correlation matrix is 241 a scalar (i.e.  $\Sigma = \sigma_1^2$ ), we use a Jeffreys prior  $(p(\sigma_i) \propto 1/\Sigma)$ . When the multi-tracer cross-covariance matrix is estimated, we specify an inverse Wishart prior distribution  $\Sigma_T \sim IW(S, \nu)$ , with a diagonal scale matrix S = I and  $\nu = 2n + 1$  degrees of freedom. A diagonal scale matrix reduces spurious correlations by penalizing tracer residuals which are not independent of each other. Spurious correlation is not a problem when the data dimension is large, but when the data are sparse such a regularization procedure is prudent (see, for instance, *Barnard et al.* [2000] or Chapter 19 in *Gelman et al.* [2003], and references therein).

Equation (8) provides the joint posterior probability of both the model parameter and the bias and covariance parameters. The marginal posterior probability of the model parameter alone is obtained by integrating the joint posterior over all other parameters:

$$p(\theta|O) = \int p(\theta, a, b, \sigma, \rho, \lambda|O) \, da \, db \, d\sigma \, d\rho \, d\lambda \,. \tag{9}$$

Since the posterior is estimated by MCMC sampling, this posterior distribution of  $\theta$  is easily obtained by simply considering the  $\theta$  samples while ignoring the samples for the other parameters.

# 3. Results

# 3.1. Effect of ocean diapynal diffusivity on the AMOC hindcasts and spatial fields

In the adopted model the AMOC strength is positively correlated with the parameters  $K_{bg}$  and  $u_{-}K_{SO}$  (Figure 1).  $K_{bg}$  has a strong influence on the model hindcasts of the maximum AMOC strength, while the AMOC sensitivity to  $u_{-}K_{SO}$  is weaker. The range of AMOC strength varies from about 5–23 Sv across all simulations. The inclusion of enhanced upper Southern Ocean mixing  $(u_{-}K_{SO}=1)$ , can increase the AMOC by a few Sverdrups, with more influence at lower  $K_{bg}$ . Under the projected climate forcings, the AMOC strength decreases in most cases, but it is more sensitive (in absolute values) to the considered forcings for higher diffusivity values. Due to the strong dependence of the AMOC structure and behavior on the values of the parameters  $K_{bg}$  and  $u_{-}K_{SO}$  in this model, a reduction in the parametric uncertainty has the potential to improve AMOC hindcast and projection in the model.

The different parameter values result in different hindcasts of ocean tracers such as CFC11 (Figure 2) and  $\Delta^{14}$ C (Figure 3), due to the different tracers advection and diffusion rates
in the model. Higher  $K_{bg}$  values result in stronger vertical water exchange, increased deep
water mass formation, which carries water with higher tracer content from the surface, and
decreased vertical stratification in the ocean.  $u_{-}K_{SO}$  broadly produces the same effects
of  $K_{bg}$ . Nevertheless,  $u_{-}K_{SO}$  impacts more heavily the lower  $K_{bg}$  runs and the Southern
Ocean stratification.

Here we analyze the tracers concentrations as vertical profiles of their averaged concentrations over the globe. We consider three different observations, CFC-11,  $\Delta^{14}C$  and
T (Figure 4, shown as an example for ENSEMBLE 1). In general, the observations are
contained by the model ensemble spread, except for T in the deep ocean, which is too
cold in the model.

### 3.2. The uncertainty of the statistical inversion

The inversion method uses the information contained in the tracers to estimate the model parameter  $K_{bg}$ , taking into account uncertainties in  $u_{-}K_{SO}$ . Key improvements 27 compared to Schmittner et al. [2009] are: (i) the estimation of the cross-correlation terms; 278 (ii) a more refined representation of structured biases in the Likelihood function; and 279 (iii) the consideration of the effects of the structural uncertainty (specifically about the 280 implementation of mixing in the SO). Here we demonstrate how these improvements affect 281 the joint posterior pdf of the model parameters. We test the sensitivity of the method to 282 the choice of the statistical (or nuisance) parameters for the distribution of  $K_{bq}$ . In this 283 sensitivity test, we do not account for uncertainties in the parameter  $u_{-}K_{SO}$ . Therefore, 284 we only use outputs from ENSEMBLE 1.

For illustration, we use two tracers,  $\Delta^{14}C$  and T, as input for the statistical inversion.

We calculate four inversion, which vary the number of statistical parameters to be esti
mated. The structure of the errors differ from each other by the representation of two

main parameters, the bias and the cross-correlation of the residuals between the model

and the observations. The bias term represents our guess of the mean function of the

residuals. We demonstrate the trade-off between complexity of the bias-correction and

the covariance structure of the residuals in this simple sensitivity study.

Specifically, we analyze four different assumptions about the structural error terms. First, we use a simple case where the bias is constant and there is no residuals cross-294 correlation; second, we use a constant bias and estimate the cross-correlation; third we 295 estimate a linear bias but no residual cross-correlation; and fourth, in which linear bias 296 and cross-correlation are both estimated. To summarize the experiments in the sensitivity 29 study, we have: a)  $\mu=b,~\rho=0,$  b)  $\mu=b,~\rho=\hat{\rho},$  c)  $\mu=az+b,~\rho=0,$  and d)  $\mu=az+b,$  $\rho = \hat{\rho}$ . Note that the calibration also estimates standard deviation, correlation length and the model parameter, as described in Section 2.3. Comparing all pdfs (Figure 5) we see that for the individual pdfs the representation of the bias term can be essential for the 301 model parameter estimation. When a more simplified bias  $(\mu = b)$  is applied (Figures 5a) and 5b), the pdfs in this example are displaced toward higher  $K_{bg}$  values, and centered on 0.3 and 0.4  $cm^2s^{-1}$ . In contrast, with the linear bias estimations, the mode of  $K_{bg}$  pdf is centered around 0.15 and 0.2  $cm^2s^{-1}$ . For the cases with linear bias (cases c and d), the standard deviation of the residuals of both tracers (Table 1) decrease in comparison 306 to the constant biases cases (cases a and b). On the other hand, the standard deviations 307 of the residuals are not influenced by the addition of cross-correlation parameters.

The inclusion of the cross-correlation parameter impacts the position of the joint posterior (black curves), and its strength is closely related to the representation of the bias. When the bias has a better representation, which is the linear bias case here (Figures 5c and 5d), the cross-correlation term has little influence on the joint pdf. A comparison of the strength of the cross-correlation parameters (cases (b) and (d) in Table 1) shows that 313  $\rho = 0.70$  when  $\mu$  is constant, and is much smaller  $\rho = 0.40$  when  $\mu$  is linear. Compar-314 ing the posteriors of the cases (a) and (b) (Figures 5a and 5b),  $\rho$  can visibly change the 315 posterior when the mean function is less structured. Case (b) shows a counterintuitive 316 result where the posterior mode is distant from the modes of the individual components 317 (Figure 5b). This result indicates that with a relatively poor representation of the mean 318 (bias) function, considering or neglecting the effects of this residual cross-correlation can 319 drastically change the  $K_{bg}$  posterior estimate. This effect becomes less pronounced, as 320 the representation of the model bias term improves (eg. Figure 5b vs. Figure 5c). As 321 discussed by Cressie [1993] (pp. 25), "What is one person's (spatial) covariance structure may be another person's mean structure". In other words, there is a trade-off between estimating a mean function for the tracer residuals to account for structural model errors and the magnitude of the residual cross correlation across the considered sources of information.

# 3.3. Estimating the uncertainty of vertical diffusivity

The analysis so far illustrates how different tracers observations can be combined to reduce uncertainty about one mixing parameter  $(K_{bg})$ . This reduction in parametric uncertainty results, at least in the framework of the adopted model, in a reduction of the prediction uncertainty about the AMOC. Of course, there are several caveats associated with structural errors and other neglected uncertainties in this study. We return to this issue in the Section 4, below. In this section we illustrate how this information can potentially be used to reduce uncertainties in two model parameters and improve model hindcasts and projections of the AMOC. Here the inversion uses our best estimate of the model bias term (linear), and accounts for cross-tracer correlation. We make three inversions (Figure 6), one to estimate  $K_{bg}$  for the ENSEMBLE 1, a second to estimate  $K_{bg}$ for the ENSEMBLE 2, and a third inversion which uses information from both ensembles to generate probability distributions for  $K_{bg}$  and  $u_-K_{SO}$  in a Bayesian model average fashion.

Information from the three considered tracers, CFC-11, T and  $\Delta^{14}C$ , is introduced in the statistical inversion for the estimation of uncertainties in the model parameters. For comparison, we also show in Figure 6 the  $K_{bg}$  pdf obtained using the climatological AMOC observations. The  $K_{bg}$  pdf is derived from estimate of the climatological AMOC strength of Lumpkin & Speer [2003] by assimilating a single data point assuming a normally distributed error. In principle, the model could be calibrated with both the ocean tracers and AMOC strength data by using the derived AMOC pdf as a prior for  $K_{bg}$ . However, this would neglect potential correlations between ocean tracer and AMOC strength residual errors. As a proper treatment of AMOC/tracer correlations is beyond the scope of this work, we present the AMOC-derived pdf just for comparison, without assimilating it in the joint posterior pdf.

The tracers distributions of both ensembles show similar behavior. Nevertheless, the ENSEMBLE 1 (Figure 6a) has in general higher  $K_{bg}$  modes in comparison to ENSEMBLE 2 (Figure 6b). This result shows that the additional mixing over the upper Southern Ocean

increases the overall magnitude of  $K_v$ , without changing  $K_{bg}$ , and tends to intensify the AMOC. The posterior pdf for  $K_{bg}$ , obtained by assimilating observations of the AMOC strength only (lines with triangles), is also displaced to lower values in ENSEMBLE 2, because ENSEMBLE 2 has stronger AMOC values for the same  $K_{bg}$  (Figure 1)

When information from both ensembles are added together (Figures 6c and 6d), the ENSEMBLE 2 dominates the Markov chain for  $\Delta^{14}C$  and T, with probabilities of 100 % and 65 % for ENSEMBLE 2, respectively. Conversely, CFC-11 has 80% probability of happening ENSEMBLE 1 (Figure 6d). The joint posterior of all tracers encompassing the two ensembles (Figure 6c) is entirely described by ENSEMBLE 2, therefore the posteriors in Figures 6b and 6c are practically identical.

When all the two model parameters are assimilated jointly (Figure 6c), the considered sources of information have rather different skill in improving  $K_{bg}$  estimates and AMOC predictions (see Table 2 for the properties of the statistical distributions).  $\Delta^{14}$ C has the highest information content with respect to improving  $K_{bg}$  estimates, its posterior 95 % credible interval (CI) is the tightest (0.21 cm<sup>2</sup>s<sup>-1</sup>) in comparison to the other tracers. CFC-11 comes in second, with a 95 % CI of 0.24 cm<sup>2</sup>s<sup>-1</sup>, and T comes last with the largest CI of 0.26 cm<sup>2</sup>s<sup>-1</sup>.

Combining the information of the three considered tracers (line with squares in Figure 6c), favors  $K_{bg}$  values in the lower part of the considered range, from 0.1–0.2 cm<sup>2</sup>s<sup>-1</sup>.

Note that the joined probability density function is narrower than each individual pdf indicating an advantage of using multiple tracer observations in reducing the parameter uncertainty.

As discussed in previous studies [e.g. Schmittner et al., 2009], the  $K_{bg}$  value in a coarse resolution ocean model represents the effects of background diffusivity combined with subgridscale diffusivity (i.e., a model shortcoming). Another shotcoming for coarse z-coordinate ocean models is the numerical diffusivity (Veronis effect), which can generate spurious diapycnal diffusion, especially in long climate simulations, in western boundary regions and regions where the isoneutral slope is large [Griffies et al., 1998, 2000]. Hence, even if our model-based estimate does not represent directly the observational estimate of pelagic diffusivity of 0.1 cm<sup>2</sup>s<sup>-1</sup> [Ledwell et al., 1993], they appear to be more consistent when we improve on the parametrization of regional mixing in the model.

# 3.4. AMOC projections

The joint posterior  $K_{bg}$  and  $u_{-}K_{SO}$  estimates (Figures 6c and 6d) can be used to derive model projections of the AMOC in 2100 and 2200 (Figure 7). The model hindcast for the maximum AMOC strength in 2000 is about 15–15.5 Sv. In 2100, the expected strength for the AMOC in this model is about 11 Sv. In 2200 the AMOC shows a slight strengthening relative to the 2100 conditions with an expected value of roughly 12 Sv. The  $K_{bg}$  and  $u_{-}K_{SO}$  estimates suggest an AMOC hindcast for the year 2000 (Figure 7)

that is about 2 Sv weaker than the climatological AMOC estimates of Lumpkin & Speer [2003]. The inclusion of the parameter  $u\_K_{SO}$  in the analysis reduces significantly the discrepancy of the AMOC estimates relative to the  $K_{bg}$  (Figure 6c). Other systematic model bias(es), such as too weak buoyancy forcing (e.g. from errors in the simulation of the atmospheric hydrological cycle and surface freshwater fluxes) can compromise the estimates of the current and projected AMOC strength for the Uvic model. Further discussion and implications are described in the next section.

### 4. Caveats

Our results are subject to many caveats. These caveats point to potentially fruitful research directions. In the statistical part, we consider only highly aggregated data. Basinwide zonal averages could, for example, provide potentially useful information on where the model performs better. In the projection part, other model parameters, such 401 as those affecting the response of the ocean-atmosphere coupled system, for example, the 402 hydrological cycle [Saenko & Weaver, 2004], climate sensitivity or sensitivity of climate 403 to aerosol concentrations, [cf. Tomassini et al., 2007; Forest et al., 2002], are also highly 404 uncertain, and can impact (probably widen) probabilistic AMOC projections and should 405 be considered. In addition, the atmospheric model in UVic is rather simplified, and 406 neglects important ocean-atmosphere feedbacks. 407

UVic does not use flux correction. Freshwater flux correction is known to improve the salinity and stratification in ocean models [Sorensen et al., 2001], and can be used to improve projections and hindcasts.

In the hindcasts part, other parameters linked to both diapycnal and isopycnal mixing may affect the structure of the AMOC. Nevertheless, according to *Jayne* [2009], tidal mixing parameters in the *St. Laurent et al.* [2002] parameterization have relatively low impact on the strength of the AMOC, and that upper-ocean wind-driven mixing may have a much stronger impact.

We show how including regional aspects of vertical mixing can improve the representation of the AMOC. The model parameters uncertainties need to be estimated together as performed here, since addition of new parameters can change the structure of the other calibrations. *Jayne* [2009] describes, "this is the typical conundrum: it is difficult to assess whether any of the given parameterizations improve the model since comparing to observational metrics may obscure compensating errors in different parameterizations".

# 5. Conclusion

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We develop and apply a computationally efficient and statistically sound method to 422 rank and quantify the skill of different sources of information to reduce the uncertainty about ocean model parameters and the resulting climate predictions. We improve on previous work by (i) refining the estimation of errors in the model structure, (ii) including 425 several ocean tracers and two model parameters at once in a computationally efficient 426 fashion, and (iii) quantifying and ranking the skill of different sources of information to 427 reduce the uncertainty about a model parameter. Subject to the aforementioned caveats, 428 we show how  $\Delta^{14}$ C, CFC-11, and T together sharpen the estimates of  $K_{bg}$  by 40 % and 429 improve AMOC projections in the UVic model. 430 The  $K_{bg}$  derived from individual observations (i.e.,  $\Delta^{14}$ C, CFC-11, T) are broadly con-431 sistent, but show slight discrepancies that we attribute predominantly to structural model 432 errors. Of the considered observations,  $\Delta^{14}$ C has the highest skill in reducing uncertainties 433 in AMOC projections, but it is also the most distant from the pdf observational derived AMOC estimates.  $\Delta^{14}C$  is followed (in decreasing skill of being able to reduce  $K_{bg}$  uncer-

AMOC strength.

AMOC projections show a reduction of the maximum of the joint posterior in 2100

tainty) by CFC-11 and T. The second parameter analyzed in this work,  $u_{-}K_{SO}$  improved

the representations of C14 and T in the model, and improves the representation of the

estimated in this study are quite similar among the considered ocean tracers and the two

by roughly 25% (3.5 Sv). Perhaps both surprisingly and encouraging, the pdfs of  $K_{bq}$ 

- ensembles analyzed, which have different different representations of the upper Southern
  Ocean mixing and AMOC. This convergence of  $K_{bg}$  estimates based on different sources
  of information and parameterizations suggest that  $K_{bg}$  can be robustly estimated from
  the oceanic tracers studied here.
- Acknowledgments. We thank Mike Eby, Damon Matthews, Bob Key and Ray Najjar for helpful discussions and feedback. This work is partially supported by the National Science Foundation as well as by the U.S. Department of Energy's Office of Science (BER) through the Northeastern Regional Center of the National Institute for Climatic Change Research. This work was partially supported by the U.S. Geological Survey. Any errors and opinions are those of the authors alone.

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# List of Figure Captions

- Figure 1. AMOC strength (Sv), defined as the maximum of the transport streamfunc-
- tion, from years 1800 to 2200. Dashed lines are for the ENSEMBLE 1 ( $u_{-}K_{SO}=0$ ); solid
- lines are for the ENSEMBLE 2 ( $u_{-}K_{SO} = 1$ ).
- Figure 2. Zonal averages for the Atlantic Ocean of CFC-11 concentration in [pmol/Kg] (colorbars) and density anomalies in [Kg/m<sup>3</sup>] (contour lines) for the model with diffusivity of  $K_{bg} = 0.05$  (top panels) and  $K_{bg} = 0.5$  (middle panels). The left column is for ENSEMBLE 1 ( $u_{-}K_{SO}=0$ ) and right column for ENSEMBLE 2 ( $u_{-}K_{SO}=1$ ). The bottom

panel shows the observations from [Key et al., 2004] and [Locarnini et al., 2006].

- Figure 3. Zonal averages for the Atlantic Ocean of  $\Delta^{14}$ C concentration in permil (colorbars) and density anomalies in [Kg/m³] (contour lines) for the model with diffusivity of  $K_{bg} = 0.05$  (top panels) and  $K_{bg} = 0.5$  (middle panels). The left column is for ENSEMBLE 1 ( $u_{-}K_{SO}=0$ ) and right column for ENSEMBLE 2 ( $u_{-}K_{SO}=1$ ). The bottom panel shows the observations from [ $K_{ey}$  et al., 2004] and [ $L_{ocarnini}$  et al., 2006].
- Figure 4. Global averaged profiles of CFC-11 [Key et al., 2004],  $\Delta^{14}$ C [Key et al., 2004] and T [Locarnini et al., 2006], for the observations (gray dots) and model ENSEMBLE 1 (colored lines). The legend for the model  $K_{bg}$  values is the same as in Figure 1.
- Figure 5. Sensitivity of the model parameter estimation to different treatments of structural model errors. Shown are the posterior probability density function of  $\Delta^{14}$ C (red lines with crosses) and T (blue lines with circles), and the joint posterior using both

observations (black line with squares). The panels are for the cases discussed in the text:

$$\text{a)} \ [\mu=b,\,\rho=0]; \ \text{b)} \ [\mu=b,\,\rho=\hat{\rho}]; \ \text{c)} \ [\mu=az+b,\,\rho=0]; \ \text{d)} \ [\mu=az+b,\,\rho=\hat{\rho}].$$

- Figure 6. Posterior probability density function of the model parameters for all considered sources of information, the joint posterior using all available information from observations (line with squares). The climatological AMOC estimate of [Lumpkin & Speer, 2003] is plotted for comparison (line with triangles). The  $K_{bg}$  estimates are for a) ENSEMBLE 1, b) ENSEMBLE 2, c) ENSEMBLE 1 + ENSEMBLE 2; d) the  $u_-K_{SO}$  estimate is for ENSEMBLE 1 + ENSEMBLE 2
- Figure 7. Joint posterior probability density function of model projections of the maximum AMOC strength in the years 2000, 2100 and 2200 using information from the  $\Delta^{14}$ C, CFC-11 and T observations. The climatological AMOC estimate of [Lumpkin & Speer, 2003] is added for comparison (line with triangles).

Table 1. Properties of the statistical distributions of the sensitivity test for the best  $K_{bg}$ : mode, bias ( $\mu = az + b$ ), standard deviation and cross-correlation of residuals for  $\Delta^{14}$ C and T, and mode of the posterior (joint distribution considering all tracers information).

Exp.	$Mode (cm^2s^{-1})$		bias (a,b)		$\sigma$		Cross-corr.	Mode of
	$\Delta^{14}C$	Т	$\Delta^{14}\mathrm{C}$	Τ	$\Delta^{14}\mathrm{C}$	Τ	at best $K_{bg}$	posterior
a)	0.3	0.4	(-14.0,0)	(0.45,0)	12.5	0.6	_	0.3
b)	0.3	0.4	(-14.0,0)	(0.45,0)	12.5	0.6	0.70	0.2
(c)	0.15	0.2	(-16.1, 9e-3)	(0.22, 3.3e-4)	7.7	0.28	_	0.15
d)	0.15	0.2	(-16.1, 9e-3)	(0.22, 3.2e-4)	7.7	0.28	0.40	0.15

Table 2. Properties of the statistical distributions (mode, mean and 95% credible interval [CI]  $(cm^2s^{-1})$ ) of  $K_{bg}$  (Figure 6c) for each considered sources of information, the posterior (joint distribution considering all tracers information), and the climatological AMOC estimate (*Lumpkin & Speer* [2003]). Also shown are the cross-tracers correlation at the best  $K_{bg}$  value estimated in the joint posterior.

Observation	Mode	Mean	95% CI	Cross-corr. at best $K_{bg}$		
				$\Delta^{14}C$	CFC-11	Т
$\Delta^{14}C$	0.15	0.15	0.22	1	0.06	0.38
CFC-11	0.20	0.23	0.26	_	1	0.02
Т	0.15	0.18	0.26	_	_	1
posterior	0.15	0.16	0.17	_	_	-
AMOC clim	0.20	0.20	0.42	_	_	-

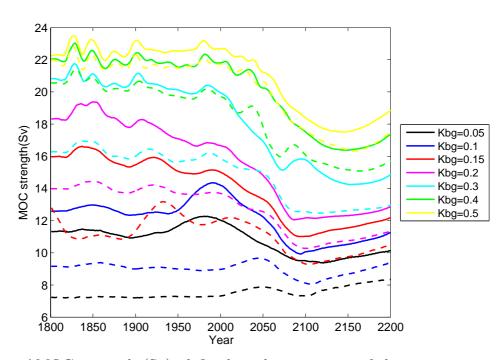


Figure 1. AMOC strength (Sv), defined as the maximum of the transport streamfunction, from years 1800 to 2200. Dashed lines are for the ENSEMBLE 1 ( $u_{-}K_{SO}=0$ ); solid lines are for the ENSEMBLE 2 ( $u_{-}K_{SO}=1$ ).

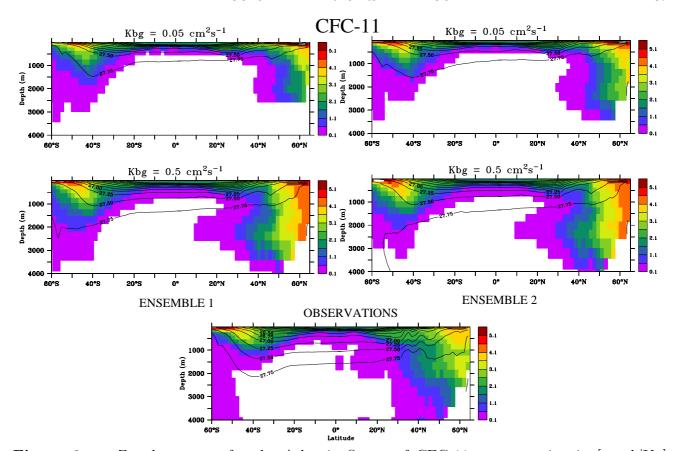


Figure 2. Zonal averages for the Atlantic Ocean of CFC-11 concentration in [pmol/Kg] (colorbars) and density anomalies in  $[Kg/m^3]$  (contour lines) for the model with diffusivity of  $K_{bg} = 0.05$  (top panels) and  $K_{bg} = 0.5$  (middle panels). The left column is for ENSEMBLE 1  $(u_{-}K_{SO}=0)$  and right column for ENSEMBLE 2  $(u_{-}K_{SO}=1)$ . The bottom panel shows the observations from  $[Key\ et\ al.,\ 2004]$  and  $[Locarnini\ et\ al.,\ 2006]$ .

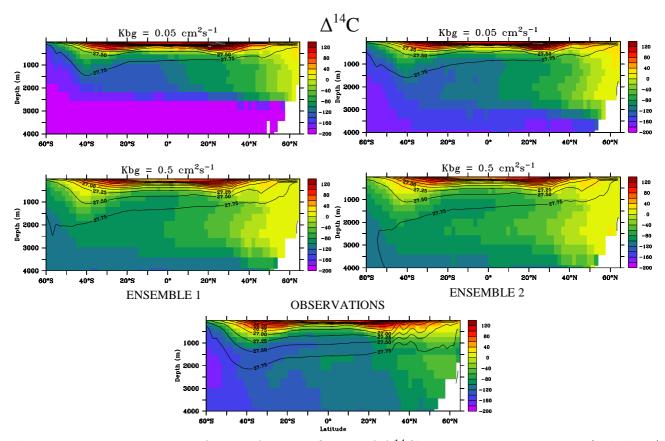


Figure 3. Zonal averages for the Atlantic Ocean of  $\Delta^{14}$ C concentration in permil (colorbars) and density anomalies in [Kg/m³] (contour lines) for the model with diffusivity of  $K_{bg} = 0.05$  (top panels) and  $K_{bg} = 0.5$  (middle panels). The left column is for ENSEMBLE 1 ( $u_{-}K_{SO}=0$ ) and right column for ENSEMBLE 2 ( $u_{-}K_{SO}=1$ ). The bottom panel shows the observations from [Key et al., 2004] and [Locarnini et al., 2006].

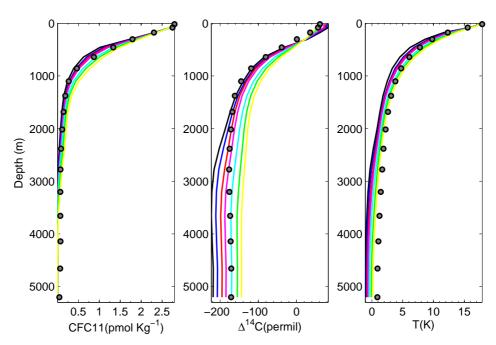


Figure 4. Global averaged profiles of CFC-11 [Key et al., 2004],  $\Delta^{14}$ C [Key et al., 2004] and T [Locarnini et al., 2006], for the observations (gray dots) and model ENSEMBLE 1 (colored lines). The legend for the model  $K_{bg}$  values is the same as in Figure 1.

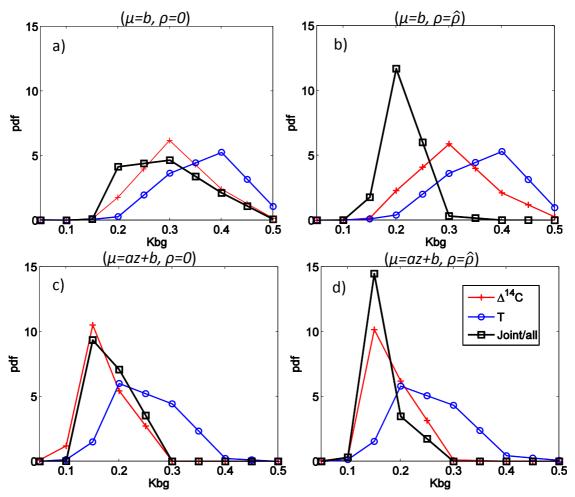


Figure 5. Sensitivity of the model parameter estimation to different treatments of structural model errors. Shown are the posterior probability density function of  $\Delta^{14}$ C (red lines with crosses) and T (blue lines with circles), and the joint posterior using both observations (black line with squares). The panels are for the cases discussed in the text: a)  $[\mu = b, \rho = 0]$ ; b)  $[\mu = b, \rho = 0]$ ; c)  $[\mu = az + b, \rho = 0]$ ; d)  $[\mu = az + b, \rho = \hat{\rho}]$ .

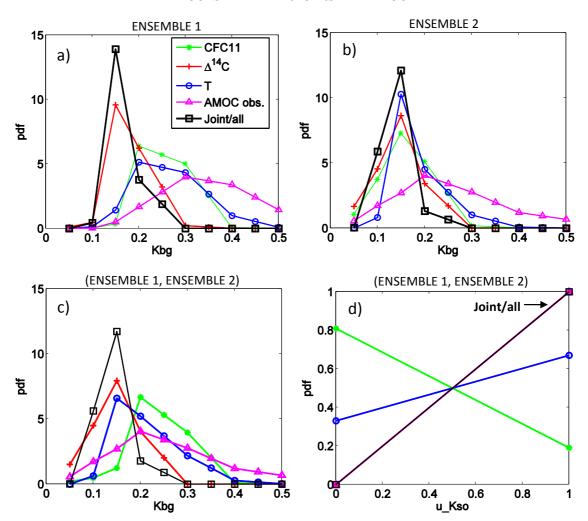


Figure 6. Posterior probability density function of the model parameters for all considered sources of information, the joint posterior using all available information from observations (line with squares). The climatological AMOC estimate of [Lumpkin & Speer, 2003] is plotted for comparison (line with triangles). The  $K_{bg}$  estimates are for a) ENSEMBLE 1, b) ENSEMBLE 2, c) ENSEMBLE 1 + ENSEMBLE 2; d) the  $u_{-}K_{SO}$  estimate is for ENSEMBLE 1 + ENSEMBLE 2

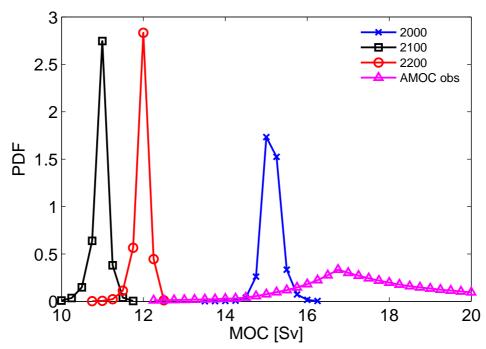


Figure 7. Joint posterior probability density function of model projections of the maximum AMOC strength in the years 2000, 2100 and 2200 using information from the  $\Delta^{14}$ C, CFC-11 and T observations. The climatological AMOC estimate of [Lumpkin & Speer, 2003] is added for comparison (line with triangles).